Predictions of Recovery of Gasoline from the LLNL Gasoline Spill Site with Dynamic Underground Stripping

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Summary

The rate of recovery of gasoline from the subsurface at a spill located on LLNL property by Dynamic Underground Stripping is controlled by a variety of thermodynamic, hydrodynamic, and mass transfer constraints. Numerical simulation of the steam injection component of dynamic stripping has been carried out to provide a first order estimate of the recovery rates. These calculations show that nearly 100% of the initial hydrocarbon is removed during the first 16 days of steam injection. However, such simulations do not accurately describe the actual mass transfer limitations expected in heterogeneous media such as that found at LLNL. A description of those mass transfer constraints is given herein. The acceleration of the mass transfer by about two orders of magnitude is expected due to increased temperatures and the de-watering of the matrix.

Numerical Simulations

A numerical simulator, M^2NOTS, has been developed for modeling three-dimensional, non-isothermal, multiphase transport of multicomponent organic contaminants in the subsurface [Adenekan, 1992]. The model utilizes the condition of thermodynamic equilibrium within each grid block control volume to evaluate the contaminant fluxes. As such, there is no provision to evaluate mass transfer constraints on any scale less than the grid spacing. Nevertheless, such calculations provide good "upper-bound" estimates of the recovery rates to be expected at LLNL during the steam injection portion of dynamic stripping.

The mesh used to simulate the steam injection is shown in Figures 1 and 2. The effectiveness of steam injection in improving the recovery rates from the high permeability zones can be evaluated by examining the response of layers 1, 3 and 4 to steam injection. The calculated percentages of each of the 3 components comprising a pseudo-gasoline (2.2% (by moles) benzene, 74.1% p-xylene, and 23.7% n-decane) recovered from the two high permeability layers initially containing gasoline (layers 1 and 3) are presented in Table 1. As shown, 100% of the hydrocarbon liquid is removed from the high permeability zones during the first 16 days of steam injection. The aqueous phase concentrations of benzene also dropped to less than 10 ppb everywhere in the high permeability zones. While the 10 ppb benzene concentration is still above regulatory limits, reductions in these benzene concentrations were being observed at the end of 16 days. These results are consistent with the experiments reported by Hunt, et al. [1988] on steam displacement of a real gasoline from a sand pack.

Mass Transfer Limitations

The removal of separate phase gasoline from regions that are not fully contacted by the flowing steam will be controlled by mass transfer from the separate phase hydrocarbon - gas interface, as illustrated in Figure 3. Two mass transfer resistances are present: the mass transfer within the liquid hydrocarbon phase and the mass transfer from the hydrocarbon - steam interface to a region where there is fresh steam flow. Past work [Ho and Udell, 1991 and Ho and Udell, 1992] has quantified these resistances and shown that the removal rates will be directly proportional to the equilibrium concentration of the least volatile compound

in the gas phase. If it is assumed that the properties of decane are representative of this least volatile compound in gasoline, then one can make estimates of the increase of the gasoline removal rate over that of vacuum extraction by evaluating the increase in the equilibrium concentration of decane in a gas mixture due to the increase in the temperature during steam injection. A graphical representation of the vapor pressures of various hydrocarbons as functions of temperature is presented in Figure 4. As illustrated in this figure, one would expect about a two orders of magnitude increase in the gasoline vaporization rate during diffusion controlled conditions due to an increase in temperature from ambient (20° C) to steam values (125° C). While this comparison is most applicable to layer 1 which is located in the vadose zone, it is also appropriate to first order for air sparging below the water table.

References

Adenekan, A. E., "Numerical Modeling of Multiphase Transport of Multicomponent Organic Contaminants and Heat in the Subsurface," PhD Dissertation, University of California, Berkeley, 1992.

Ho, C. K. and Udell, K. S., "An Experimental Investigation of Air Venting of Volatile Liquid Hydrocarbon Mixtures from Homogeneous and Heterogeneous Porous Media," *J. Contaminant Hydrology*, (In Press) October, 1992.

Ho, C. K. and Udell, K. S., "A Mass Transfer Model for the Removal of a Volatile Organic Compound from Heterogeneous Porous Media During Vacuum Extraction," *Heat Transfer in Geophysical Media*, ASME HTD-172, July, 1991.

Hunt, J. R., Sitar, N., and Udell, K. S., "Non-Aqueous Phase Liquid Transport and Cleanup, Part II. Experimental Studies," *Water Resources Research,* 24, No. 8, pp. 1259-1269, August, 1988.

Table 1. Calculated percentage of initial mass of each hydrocarbon component removed during steam injection for 16 days at the LLNL gasoline spill site (from *Adenekan* [1992]).

	Layer 1			Layer 3		
	gas	water	NAPL	gas	water	NAPL
Benzene	77.7%	20.3%	2.0%	55.8%	22.1%	22.1%
p-Xylene	96.4%	1.8%	1.8%	84.9%	2.0%	13.1%
n-Decane	98.4%	0.0%	1.6%	90.5%	0.0%	9.5%

Depth (m)

Ground Surface

0

Heat loss to overburden

24

Layer 1

32

Layer 2

37

Layer 3

Layer 4

40

Heat loss to underburden

Water Table

Injector

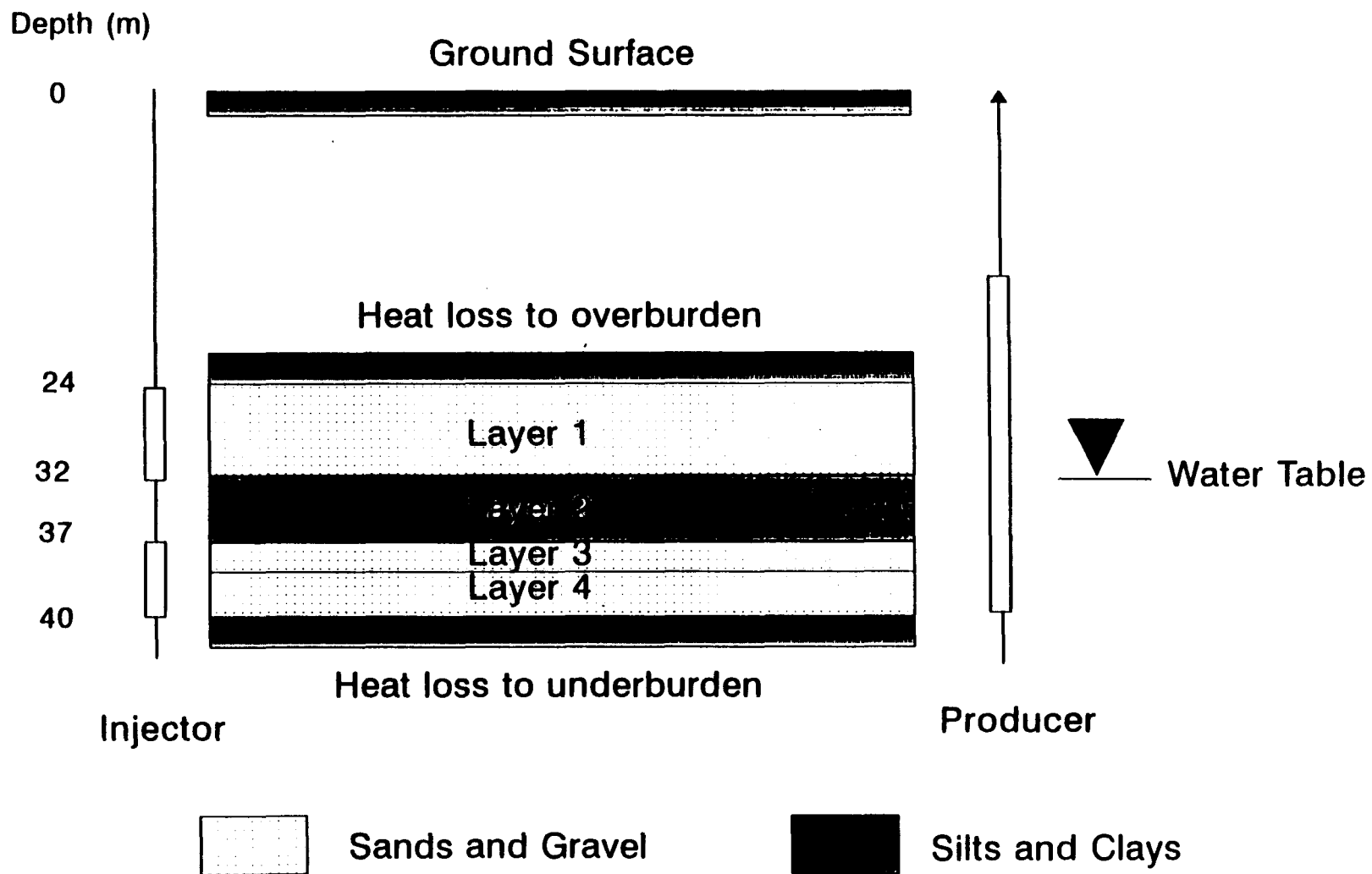Producer

Sands and Gravel

Silts and Clays

Figure 1. Vertical section of the discretized layers representative of the
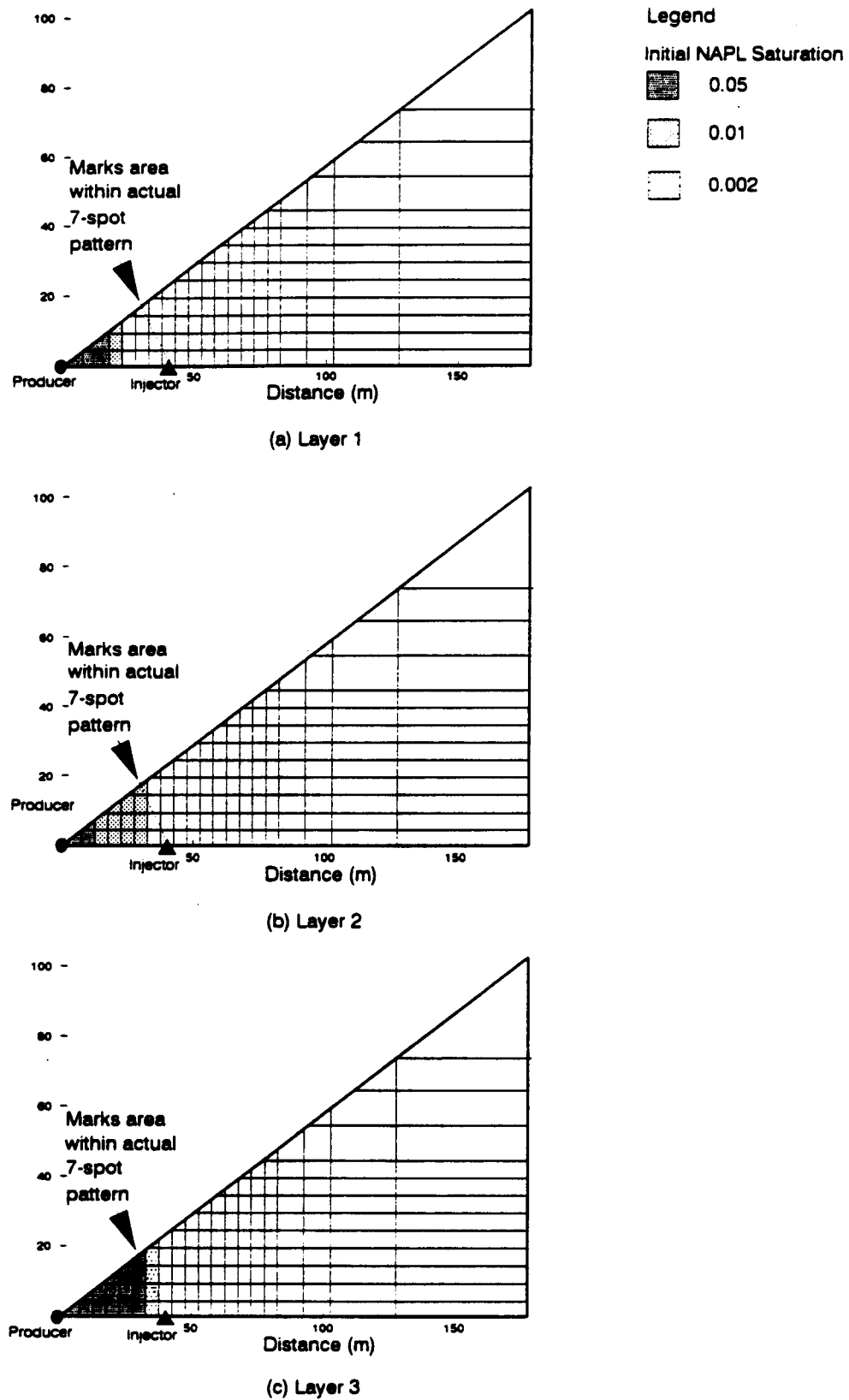LLNL gasoline spill (from *Adenekan* [1992]).

Figure 2. Plan view of the discretization and non-aqueous phase liquid hydrocarbon (NAPL) distribution in layers 1, 2, and 3 (from *Adenekan* [1992]).
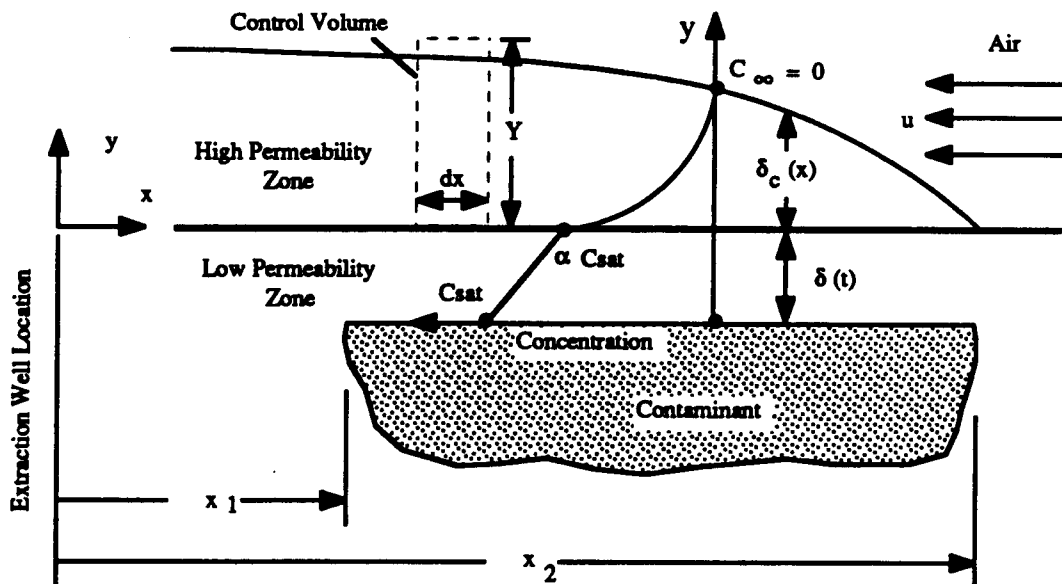
Figure 3. Schematic model of a pool of liquid hydrocarbon receding
from the top surface during mass transfer limited vaporization
(from *Ho and Udell* [1992]).

Vapor Concentrations of Various Hydrocarbons Vs. Temperature(Pv<101.32
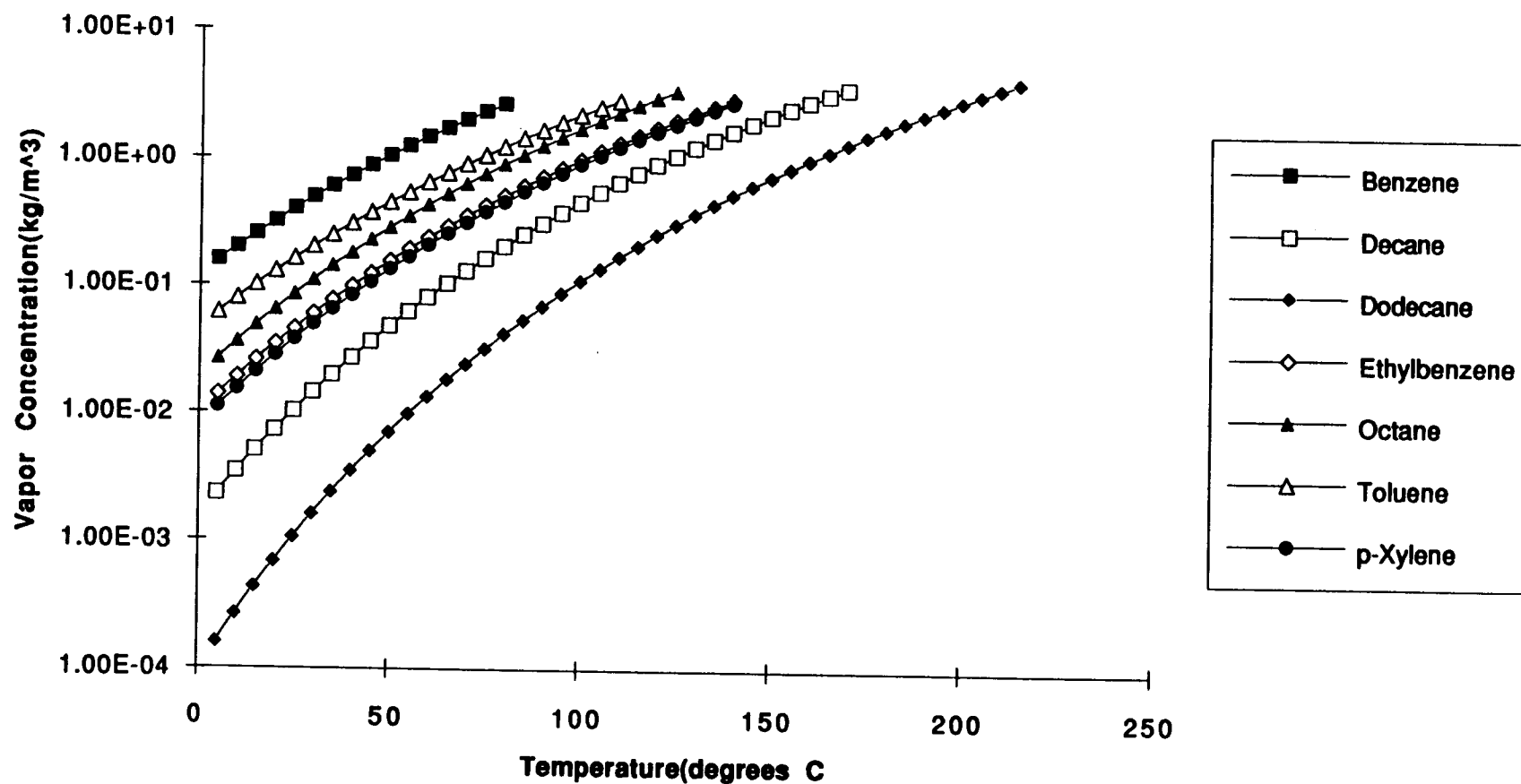

Figure 4. Equilibrium vapor concentrations of various hydrocarbons in a
gas mixture at one atmosphere as functions of temperature.